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ÚSTAV FYZIKÁLNÍHO INŽENÝRSTVÍ

FACULTY OF MECHANICAL ENGINEERING
INSTITUTE OF PHYSICAL ENGINEERING

IMPROVEMENT OF CONTROL AND ANALYSIS TECHNIQUES OF A SPM MODEL

ZDOKONALENÍ ŘÍDÍCÍCH A ANALYZAČNÍCH TECHNIK VÝVOJOVÉHO MODELU SPM

BAKALÁŘSKÁ PRÁCE
BACHELOR'S THESIS

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ZADÁNÍ BAKALÁŘSKÉ PRÁCE

student(ka): Marcel Štefko

který/která studuje v **bakalářském studijním programu**

obor: **Fyzikální inženýrství a nanotechnologie (3901R043)**

Ředitel ústavu Vám v souladu se zákonem č.111/1998 o vysokých školách a se Studijním a zkušebním řádem VUT v Brně určuje následující téma bakalářské práce:

Zdokonalení řídících a analyzačních technik vývojového modelu SPM

v anglickém jazyce:

Improvement of control and analysis techniques of a SPM model

Stručná charakteristika problematiky úkolu:

Macroscopic models of scanning probe microscopes find applications not only in pop-science lectures, but also in scientific work. Using suitable analogies, we can observe the behaviour of the enlarged tip and specimen, and thus better understand the underlying physical principles of SPM. Processing of data from an enlarged probe is practically identical to real scanning probe microscopes. This can be used to develop electronics or control software for SPM.

Cíle bakalářské práce:

1) Study current macroscopic analogies of different SPM techniques.

2) Implement a chosen analogy into the SPM model.

3) Integrate a single-board computer which will allow to control the model without connecting an external computer into the system.

Seznam odborné literatury:

[1] Horowitz, Paul. The art of electronics. 2nd ed. New York: Cambridge University Press, 1989, xxiii, 1125 s. ISBN 05-213-7095-7.

[2] Binnig, G.; Rohrer, H.: Scanning tunneling microscopy. Helvetica Physica Acta, Volume 55, 1982: s. 726{735, ISSN 0018-0238.

[3] Meyer, E.; Hug, H. J.; Bennewitz, R.: Scanning Probe Microscopy: The Lab on a Tip. Advanced Texts in Physics, Springer, 2004, ISBN 9783540431800.

Vedoucí bakalářské práce: Ing. Dalibor Šulc

Termín odevzdání bakalářské práce je stanoven časovým plánem akademického roku 2014/2015.

V Brně, dne 20.11.2014

L.S.

prof. RNDr. Tomáš Šikola, CSc. Ředitel ústavu	doc. Ing. Jaroslav Katolický, Ph.D. Děkan fakulty

Abstrakt
Bakalářská práce se zabývá zdokonalováním výukového modelu mikroskopu atomárních sil (AFM). Součástí práce je rešerše stávajících analogii mezi makroskopickými jevy a fenomény spojenými s mikroskopii rastrovací sondou. Dále byla vybrána vhodná analogie, která byla následně implementována do již existujícího modelu mikroskopu atomárních sil. Do modelu byl integrován i jednodeskový počítač, který zajistí ovládání i bez nutnosti připojení externího počítače. Na závěr byly vyhodnoceny vlastnosti použité sondy a analogie mezi modelem a skutečnými mikroskopy atomárních sil.

Summary
This Bachelor Thesis is focused on development of a model of an atomic force microscope (AFM). First part of the thesis is research of already existing analogies between macroscopic phenomena and phenomena connected to scanning probe microscopy. A suitable analogy was chosen and implemented into an existing AFM model. A single-board computer was integrated into the model to enable control without connecting an external computer. In final chapters, probe behaviour and analogies between the model and real atomic force microscopes are discussed.

Klíčová slova
Mikroskopie rastrovací sondou, SPM, mikroskopie atomárních sil, AFM, model, analogie

Keywords
Scanning Probe Microscopy, SPM, Atomic Force Microscopy, AFM, model, analogy

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I declare that I have developed and written the enclosed Bachelor Thesis completely by myself, and have not used sources or means without declaration in the text. Any thoughts from others or literal quotations are clearly marked. The Bachelor Thesis was not used in the same or in a similar version to achieve an academic grading or is being published elsewhere.

Marcel Štefko

I would like to thank my supervisor Ing. Dalibor Šulc for his invaluable advice, patience and helpfulness during development of this Bachelor Thesis. I would also like to thank all academic staff of the Institute of Physical Engineering at Brno University of Technology for their exemplary approach to teaching and motivating their students. I also thank my schoolmates and all other friends for our time spent together. Foremost, I would like to thank my parents and family for supporting me not only in my studies, but all aspects of my life.

Venované rodičom.

Marcel Štefko

Contents

1. Introduction

"If you can't explain it simply, you don't understand it well enough." This quote[1] encapsulates the importance of the ability to clearly and comprehensibly explain complex phenomena and subjects to the general public. This ability is equally important for both the "student" and the "teacher".

For the students, getting the subject explained to them in a way they can understand is vital. A good lecturer is one who is not "detached from reality", and can adjust the level of the lecture to the level of the audience. A good lecturer finds balance between rigorousness and simplicity. Where possible, the subject should be explained using appropriate analogies and demonstrations. Just as a picture is worth a thousand words, a demonstration is worth a thousand explanations.

The teacher also benefits greatly from this process. Explaining a subject requires thorough understanding, and often helps you identify areas, where your knowledge might be not as adequate as you have previously thought. This phenomenon is the foundation of an effective study method – explaining it to your dog.[2]

Creating a demonstration of a phenomenon takes this even further. It forces you to think about the subject from a different perspective. Often, you can not demonstrate it directly, but have to find appropriate analogies, which make the subject easier to convey, but do not distort it too much in the process. Explaining and demonstrating complex subjects is not an easy task, and people who master it are hard to find and highly regarded. Richard Feynman's lectures on physics have become legendary for their "simplicity, beauty and unity". Walter Lewin's lectures from MIT have also been accessed by millions of people worldwide, many of whom would never have taken an interest in these subjects otherwise. Getting the general public interested is beneficial for the whole scientific community.

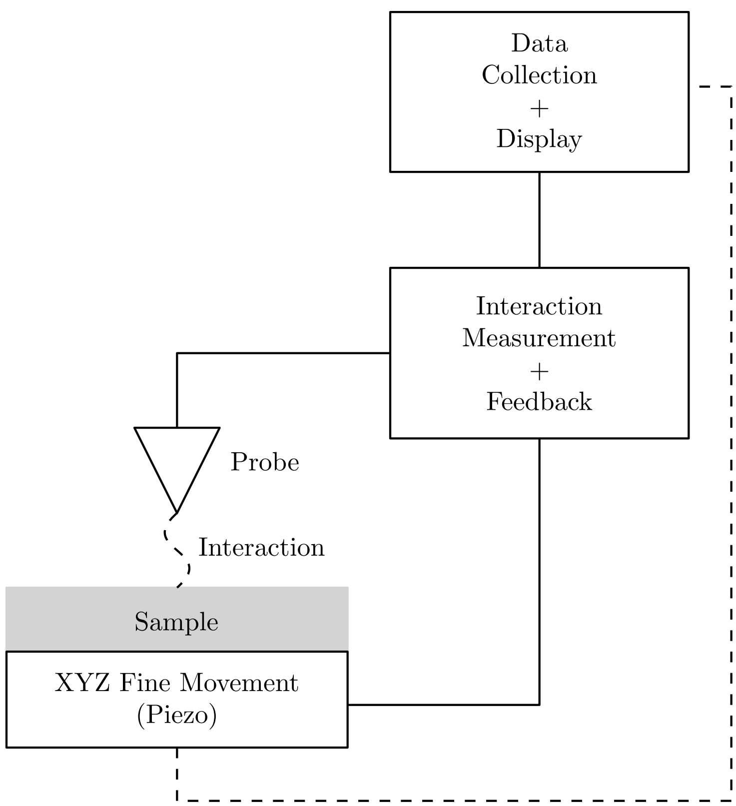
Subject of this work is development of a model of a scanning probe microscope. In the first part (Chapters 2 – 4), various scanning probe microscopy techniques – and appropriate analogies to them – are discussed. In the second part (Chapters 5 – 10), a suitable technique is chosen and implemented into an already existing model.

[1] Often misattributed to Albert Einstein or Richard Feynman, although the real author is unknown.
[2] Younger siblings or inanimate objects such as plants are also popular victims.

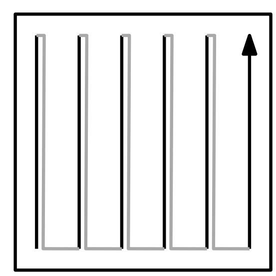
2. Scanning Probe Microscopy

2.1. Introduction

Scanning probe microscopy is a term used to describe a wide variety of techniques used to inspect various properties of surfaces, such as topography, conductivity, magnetic properties, and many more, on the atomic scale using a physical probe. Ever since its invention in 1982, SPM has become a popular tool for scientists and engineers trying to better understand molecular interactions and manipulate matter on the scale of individual atoms. Availability of high-quality instruments and relative ease to adapt these techniques to a wide range of conditions is also an important factor contributing to its popularity and spread across many branches of scientific research. [1]



(a) Generalised schematic.



(b) Top view of probe movement across the sample.

Figure 2.1: Principle of SPM function. While the type of interaction being measured, probe characteristics, feedback type and data display can vary greatly, this general principle is common for all. [2]

2.2. Imaging

To form images of the surface, the SPM scans the surface,[1] usually using piezoelectric actuators, which can be located either under the sample, or attached to the probe. The data is collected by a computer and then visualised in false color or a 3-dimensional plot.

2.3. Variations

There is a wide variety of interaction types between the probe and the sample that can be used for SPM. Some of the most well-known and commonly used are:[2]

- Quantum tunnelling effect - scanning tunnelling microscopy (STM).
- Atomic forces - atomic force microscopy (AFM).
- Magnetic forces - magnetic force microsopy (MFM).
- Electrostatic capacitance - scanning capacitance microscopy (SCM).
- Near-field optics - scanning near-field optical microscopy (SNOM).

2.4. Operation modes

2.4.1. Setpoint and feedback

A setpoint in control theory is a desired value of a variable of a system. Usually, a feedback loop is implemented into the system, to return this variable to its original value, if it departs from this value due a perturbation. [4]

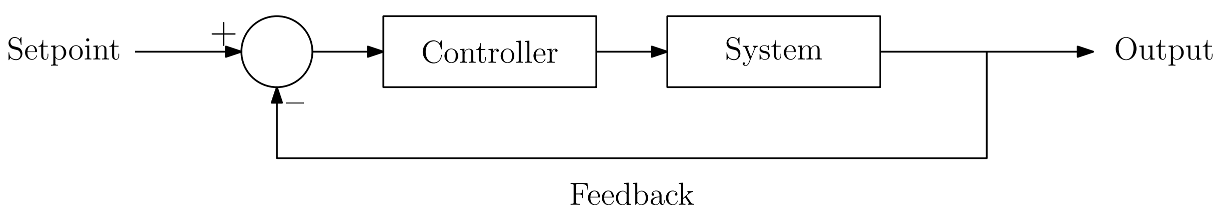


Figure 2.2: A generalized feedback loop.

2.4.2. Feedback in SPM

For every SPM technique, the feedback loop can operate in two distinct modes - constant height mode, and constant interaction mode.[3]

[1] That is, it moves across the surface in a pattern similar to the way your eyes travel over the page while reading this text, and takes measurements of the interaction at each point of a virtual rectangular grid spread across the surface - see Figure 2.1b.

[2] This list is by no means exhaustive. There are many more types or slight variations of SPM techniques, and new ones are constantly being developed, even more than 30 years after invention of the first one. [3]

[3] The latter is also often referred to as constant *force* mode, although the interaction being measured does not necessarily have to be a force.

In constant height mode, the height of the probe is kept constant during the scan, and changes in interaction are measured and recorded. In constant interaction mode, the feedback loop maintains the interaction at a certain level, and adjusts the height of the probe accordingly. [5]

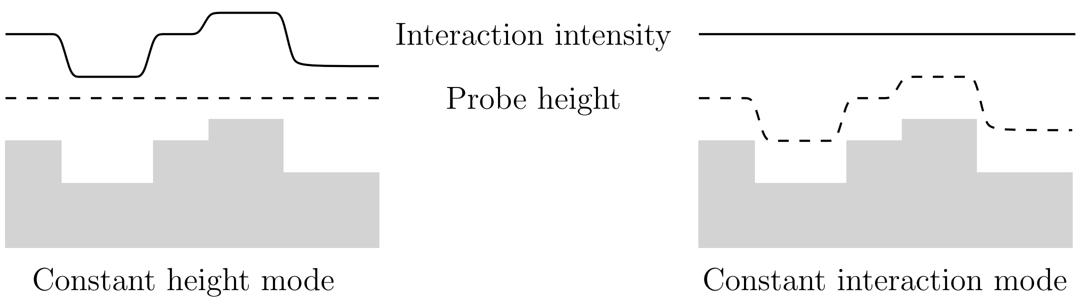


Figure 2.3: Comparison of constant height and interaction mode. The dashed line marks the height of the probe as it scans the surface, the solid line represents intensity of interaction.

3. Analogies to SPM phenomena

3.1. The Fridge Magnet Experiment

This method can be used to demonstrate the basic principle of SPM - forces acting on a probe moving across the specimen surface. Its main advantages are extremely low costs and preparation time. These factors make it ideal for use in middle/high school classrooms, or as do-it-yourself challenges for children interested in science.

This experiment is based on the attraction and repulsion of opposite, respectively equal poles of any magnets. A fridge magnet can have several possible distributions of poles across its area – see Figure 3.1. It is impossible to identify these distributions by sight or touch, but using a thin strip of another fridge magnet as a probe, and moving it across the surface can help identify the pattern. [6]

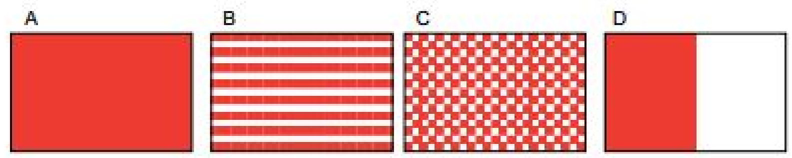


Figure 3.1: Possible distributions of magnetic poles or a fridge magnet across its surface. Red - north, white - south. Image adapted from [6]

When the "probe" is moved a small distance above the magnet, the tip of the probe gets attracted or repulsed from the surface, depending on the configuration of poles directly under it.[1]

3.2. The Scanning Theremin Microscope

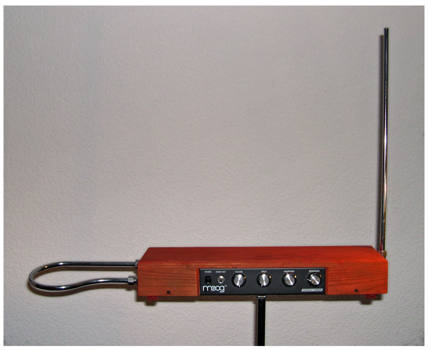
The Scanning Theremin Microscope[2] was developed at the University of Notre Dame to introduce and demonstrate SPM methods to broad audiences at low costs. It uses a capacitance proximity probe, which produces oscillations in the audible range of frequencies, in response to close presence of physical objects. The same principle is used in a musical instrument - the theremin.

> "Capacitance, by definition, is the ability of an object to store electric charge. This can be measured by delivering charge to the object at a fixed rate (a constant current) and measuring the resulting potential versus time. A large capacitance describes a system that charges up slowly, whereas a small-capacitance system charges up quickly. When playing the theremin, the musician's hand is incorporated into the electrical circuit, causing small changes in capacitance.
>
> Linking the pitch antenna to an oscillator circuit results in a frequency for this oscillator that is dependent on hand position: capacitance is larger when

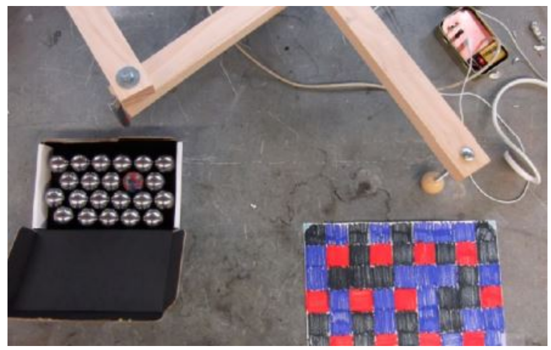
[1] This principle is effectively the same as the principle of all SPM methods. The only thing that changes is the physical property which is measured. In this case, it is the magnetic force.

[2] Not to be confused with the Scanning Thermal Microscope, as they share the same acronym (SThM).

a hand is close to the antenna, resulting in a longer charging time and a lower frequency. This is the variable oscillator, and its frequency is measured with respect to an unchanging local oscillator by mixing the two signals together to obtain a beat (heterodyne) signal. Circuits originally used for the theremin employed oscillators with frequencies in the range of tens to hundreds of kilohertz. Hand position would change the frequency of the variable oscillator by parts per hundred or parts per thousand, resulting in a beat frequency in the acoustic range, $\sim$10$-$1000 Hz." [7]



(a) Musical instrument. Image source: [8]



(b) Scanning Theremin Microscope. Image source: [7]

Figure 3.2: The Theremin.

The probe, as in the previous example, is slowly moved across the scanned area. Changes in distance between the surface and the probe result in change of pitch of produced sound. This makes it especially attractive for classroom demonstrations. The probe position - pitch relation has to be recorded either entirely manually, or using a pantograph – Figure 3.2b.

It is also easy to create new samples for measuring, as materials such as metals or modelling clay produce a large response in change of pitch.

3.3. Macroscopic mechanical model

The simplest way to demonstrate the principles of Scanning Probe Microscopy, is simply to “upscale” the microscope. Piezoelectric scanners can be replaced with linear stepper motors, the cantilever probe can be enlarged to suitable dimensions,[3] and its flexion can be measured in various ways, for example using a magnet attached to the cantilever and a stationary Hall probe, or a tensometric bridge, or a laser reflected to a diode array, as in original SPM. Various methods which can be demonstrated on this type of model, and also the analogies which are used, are discussed in next chapter.

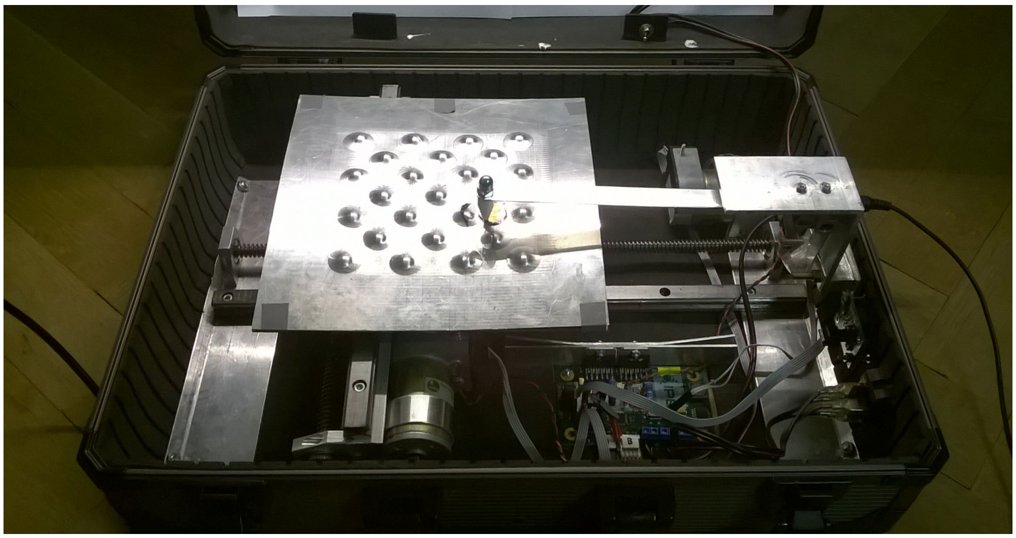


Figure 3.3: Macroscopic model of a scanning probe microscope.

[3] Although maintaining all dimensions and distances exactly to scale might not be possible, as is explained in the next chapter.

4. Analogies to different SPM techniques

4.1. Scanning Tunnelling Microscopy

4.1.1. The technique

The scanning tunnelling microscope is the oldest type of a scanning probe microscope, and its invention earned its creators Gerd Binning and Heinrich Rohrer the Nobel prize in physics in 1986. It was the first instrument to provide real images with atomic resolution. [9]

The STM uses the quantum tunnelling effect to induce a small, but measurable current between the sample and the probe tip, which is usually only one atom thick at its end. For the tunnelling effect to occur, both the probe and the sample must be made from conducting materials. [10]

The tunnelling effect exhibited in STM can be approximated as an electron tunnelling through a 1-dimensional rectangular potential barrier, with the transition probability P given as:

$$P(d) = e^{-2\kappa d}, \tag{4.1}$$

where d is the width of the barrier and κ is a constant dependent on the energy of the electron and the height of the potential barrier.

Due to the exponential relation between the probability of an electron tunnelling through the barrier and the barrier width, the tunnelling current also depends exponentially upon the distance between the sample and the probe. This is the reason why STM is so sensitive - a small change in the distance can result in a large change in current. [10]

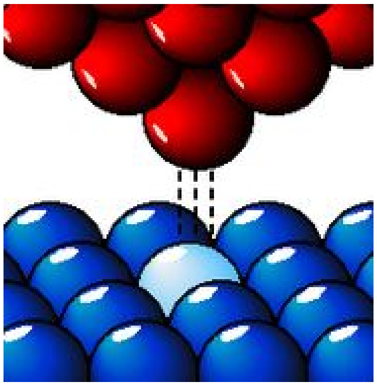
STM is especially useful when trying to determine the electronic properties of a surface with high resolution. On the other hand, if you want to map actual topography of a surface, you can encounter some issues. For example, a region of the surface can be oxidised and thus the STM will report a change in current even though the distance hasn't actually changed. It can result in incorrect readings or even the probe digging into the sample.

4.1.2. The analogy

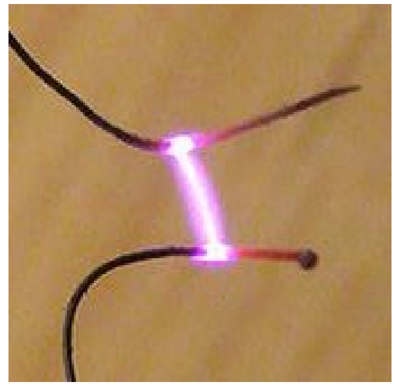
Although there is no classical or macroscopic analogy to the quantum tunnelling effect, some similarities could be found between quantum tunnelling and electric arc discharge. If there exists a difference in electric potentials between a sample and probe, a dielectric between them acts as an insulator, until the distance between them d is low enough for dielectric breakdown to occur. In air, the voltage between the sample and the probe has to be greater than breakdown voltage U [11]:

$$U(d) = kd \tag{4.2}$$

where $k = 3\,\mathrm{kV\,mm^{-1}}$ is the dielectric strength of air and d is the distance between the probe and the sample.



(a) Quantum tunneling in STM. Source: [8]



(b) Electric arc. Source: [8]

Figure 4.1: Analogy between quantum tunnelling and electric arc discharge effects.

There are some key differences between the principle of STM and this analogy. First of all, the relationship is not exponential, but linear. Also, once discharge occurs, it is necessary to stop it before making another measurement, either by increasing the distance or reducing voltage.

Both modes of STM can be demonstrated using this model. The constant height mode can be achieved by keeping the probe at a certain height, and at each point of the scan raster, the voltage between the probe and the sample is increased, until discharge occurs. This discharge voltage can then be correlated with the distance between the probe and the sample, using equation (4.2). The constant current mode works similarly, but this time the voltage is kept constant and the height of the probe above the sample is slowly decreased at each scan point, and again the height at which discharge occurs can be correlated to the distance between the probe and the sample by equation (4.2).

A good demonstration of precision with which STM operates is, that if you would want to preserve the relationship between vertical resolution and probe dimensions, the probe the size of the Eiffel tower would have to move 1 mm above the surface with an accuracy of 1 µm.[1] [12]

Main drawbacks of this model are, that voltages required for it to work are in the order of kilovolts, and pose a danger of electric shock to people who accidentally touch it. This makes the model dangerous, especially for children, and thus it is unsuitable for demonstrations in schools.

4.2. Contact AFM

4.2.1. The technique

Atomic force microscopy is based on measurement of atomic forces acting on the scanning probe tip close to the surface of the specimen. These forces are usually measured by measuring the flexion of the cantilever, which deforms itself under these forces. The flexion can be measured in different ways, for example using a laser reflected from the cantilever to a diode array, or using a Michelson interferometer.

[1] Not only would this be extremely hard to implement, it would also be counterproductive as the objective is to make all processes – including vertical probe movement – visible to human eyes.

These atomic forces are often approximated by the Lennard-Jones potential, which combines attractive van der Waals and repulsive quantum-mechanical interactions [5]:

$$w(r) = 4w_0 \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right], \tag{4.3}$$

where r is the distance between atoms of the surface and the tip, w_0 is the minimal value of potential energy and σ is the equilibrium distance of the two atoms. By taking the negative derivative of this potential with respect to distance, we obtain the force of this interaction:

$$F = -\frac{\mathrm{d}w}{\mathrm{d}r} = 24w_0 \left(\frac{2\sigma^{12}}{r^{13}} - \frac{\sigma^6}{r^7} \right). \tag{4.4}$$

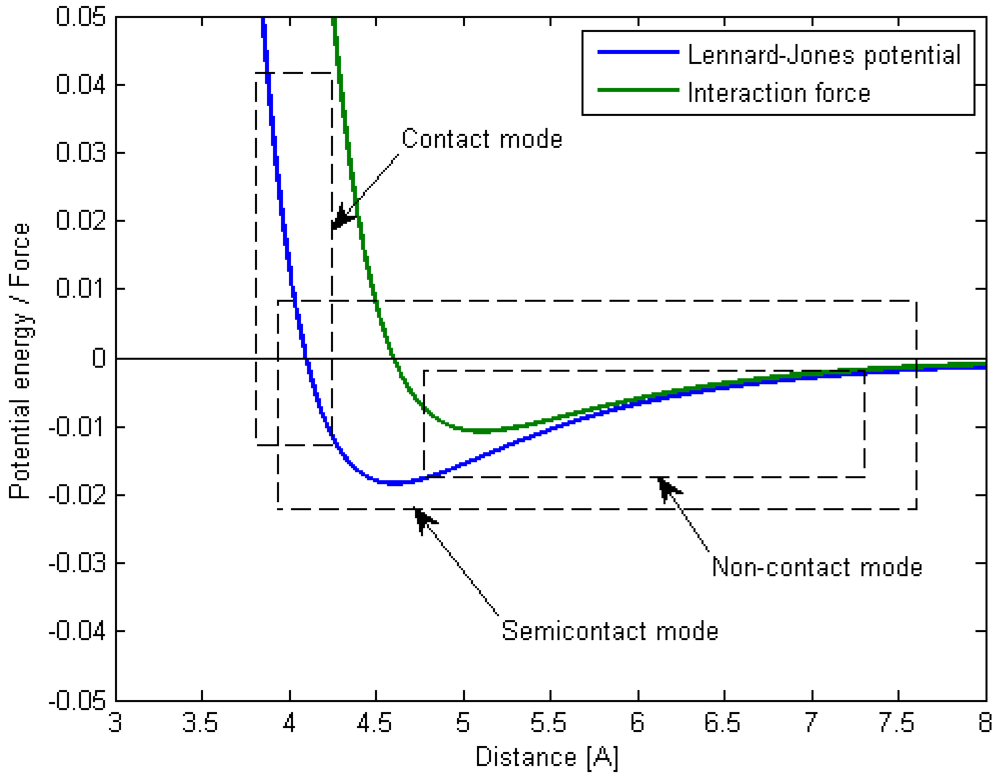


Figure 4.2: Lennard-Jones potential and its interaction force for two atoms. Approximate areas of operation of different AFM modes are marked by dashed rectangles. Vertical axis units are arbitrary.

In contact mode, the tip is in permanent contact with the specimen, and the forces acting on it are repulsive and relatively big (in the order of 10^{-7} N). From measurement of these forces, either in constant force mode, or constant height mode, topography of the specimen can be determined.

4.2.2. The analogy

Analogy to contact AFM mode is quite straightforward. The whole system is simply upscaled, and the probe comes into direct contact with the specimen. Flexion of the cantilever is measured, and correlated with height of the sample at point of contact. Both constant force mode and constant height mode can be easily demonstrated.

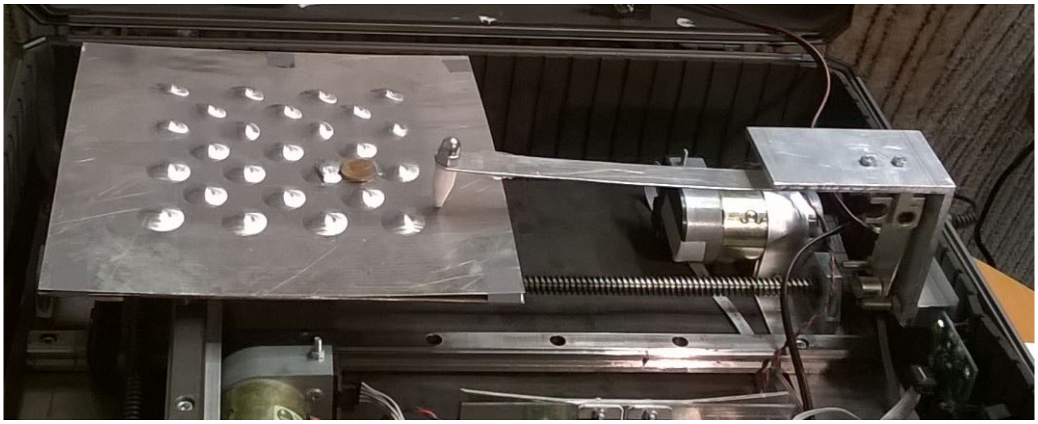


Figure 4.3: Demonstration of contact mode of AFM.

4.3. Non-contact AFM

4.3.1. The technique

In non-contact AFM mode, the tip of the probe never comes into contact with the sample. Instead, the tip of the probe oscillates at or close to its resonant frequency at a distance of $50 - 100\,\mathring{A}$. The attractive van der Waals forces at this distance are in the order of $10^{-9}\,\mathrm{N}$ [5]. These forces, which act on the oscillating probe, cause changes in resonant frequency, amplitude and phase of the oscillations. These changes can be detected and distance of the probe and sample can be determined.

Its advantage is low risk of damage, because the sample and the probe never come into contact. On the other hand, measurements can be affected by presence of a contamination layer on the surface of the sample, which can fill in nanostructures and make them harder to detect, or cause other unwanted forces (i.e. viscosity). [5]

This technique can be also applied to other than van der Waals forces, for example electrostatic, magnetic or chemical interactions .

4.3.2. The analogy

Finding an analogy to this method is problematic for several reasons. You have to find a suitable force which acts over macroscopic distances (in the order of centimetres). Gravitational force is too weak to be detectable. Electrostatic or magnetic force are good candidates, but both have drawbacks.

In case of the electrostatic force, both the sample and the tip have to be electrically charged, which brings problems already mentioned in Section 4.1.2. With magnetic force, finding materials with suitable magnetic properties for the probe and the sample can be problematic, especially in close vicinity of unshielded electronic equipment which can be damaged. In both cases, the oscillating probe would cause electromagnetic induction due to Faraday's law, which would also have to be taken into account.

4.4. Semicontact AFM (tapping mode)

4.4.1. The technique

Semicontact AFM mode combines features of previous two modes. The probe oscillates as in non-contact mode, but comes into contact with the sample in each cycle. Its benefits are, that vertical movement of the probe almost completely eliminates lateral forces and thus reduces the risk of probe or specimen damage as opposed to contact mode. Furthermore, every cycle it breaches the contamination layer, and allows for direct measurements of the sample surface. These two properties explain the popularity of semicontact AFM [5].

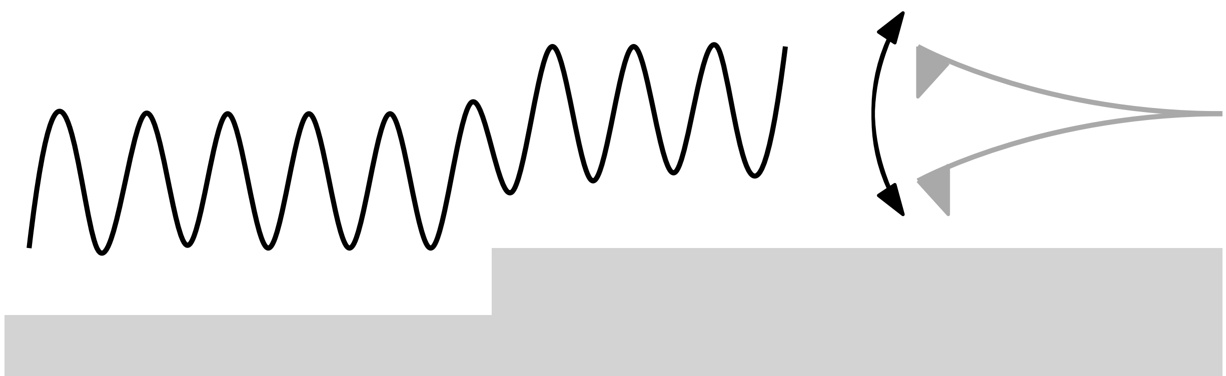


Figure 4.4: Semicontact mode of AFM (constant amplitude mode).

In this mode, the probe oscillates with a large amplitude ($10-100\,\mathrm{nm}$). When it comes into contact with the sample, this amplitude is reduced, and additionally, the oscillations are phase-shifted. Both the amplitude change and phase shift can be used to determine properties of the sample.

4.4.2. The analogy

Semicontact AFM mode is arguably easier to implement in a macroscopic model. Oscillations of the cantilever, although at much lower frequencies due to increased dimensions, can be invoked in various ways, such as using a sound speaker, or an electrical coil and a magnet, etc. The oscillating tip will literally tap the surface, which will cause both change in amplitude and phase shift.

5. Objectives

The objective of this thesis is to improve the already existing model of a scanning probe microscope, built at the Institute of Physical Engineering of Brno University of Technology, with the purpose of easier and more interesting demonstration of SPM techniques to the general public at science fairs and similar events. This objective can be split into two separate tasks:

1. Implement a new suitable SPM technique into the model.
2. Remove the need for a computer with special software by integrating a single-board computer into the model.

5.1. New SPM technique implementation

Since the model only supported constant height AFM contact mode (described in Section 4.2), it would be beneficial to implement a way to also demonstrate the difference between constant height and constant interaction modes described in Section 2.4. For this, the probe is needed to be able to move vertically, which requires considerable changes in both construction and electronics of the model.

If this technique is implemented successfully, the model can be further modified to support semicontact mode described in Section 4.4. This will also require a way to induce oscillations of the cantilever.

5.2. Single-board computer integration

The model was originally developed to be controlled by an external computer running Windows OS, so its controlling software was programmed in C# and .NET user environment. This is unfortunately unsuitable for a single-board computer, since these are not able to natively run .NET software.[1]

This means that the control software has to be ported to a different, preferably more open and flexible language.

[1] With the introduction of Windows 10 to Raspberry Pi model 2, this may change in the future. An open-source alternative (Mono) of course exists, but is not complete and often unreliable.

6. Function

Original function schematic of the SPM model is described in Figure 6.1.

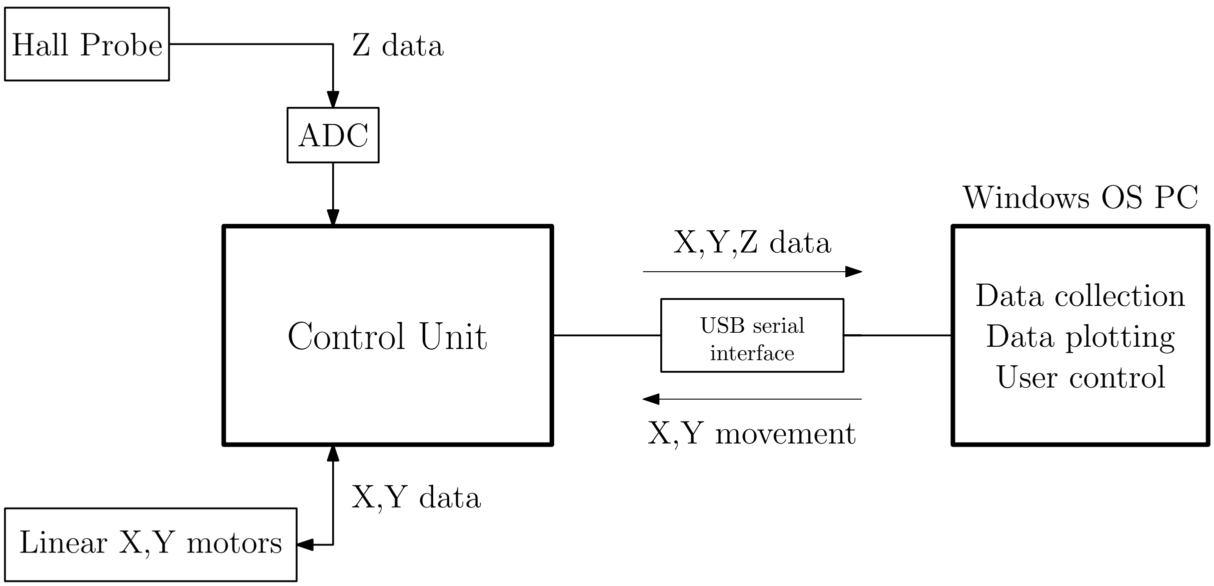


Figure 6.1: Schematic of the original model. A Windows OS computer with control software installed communicates via a USB serial interface with the Control unit, which controls movement of the sample under the probe and gathers information of probe height from the Hall probe.

This relatively simple design had to be innovated to allow implementations of multiple scanning modes, which require movement of cantilever in vertical axis and induction of oscillations of the cantilever. Schematic of new design of the model is depicted in Figure 6.2.

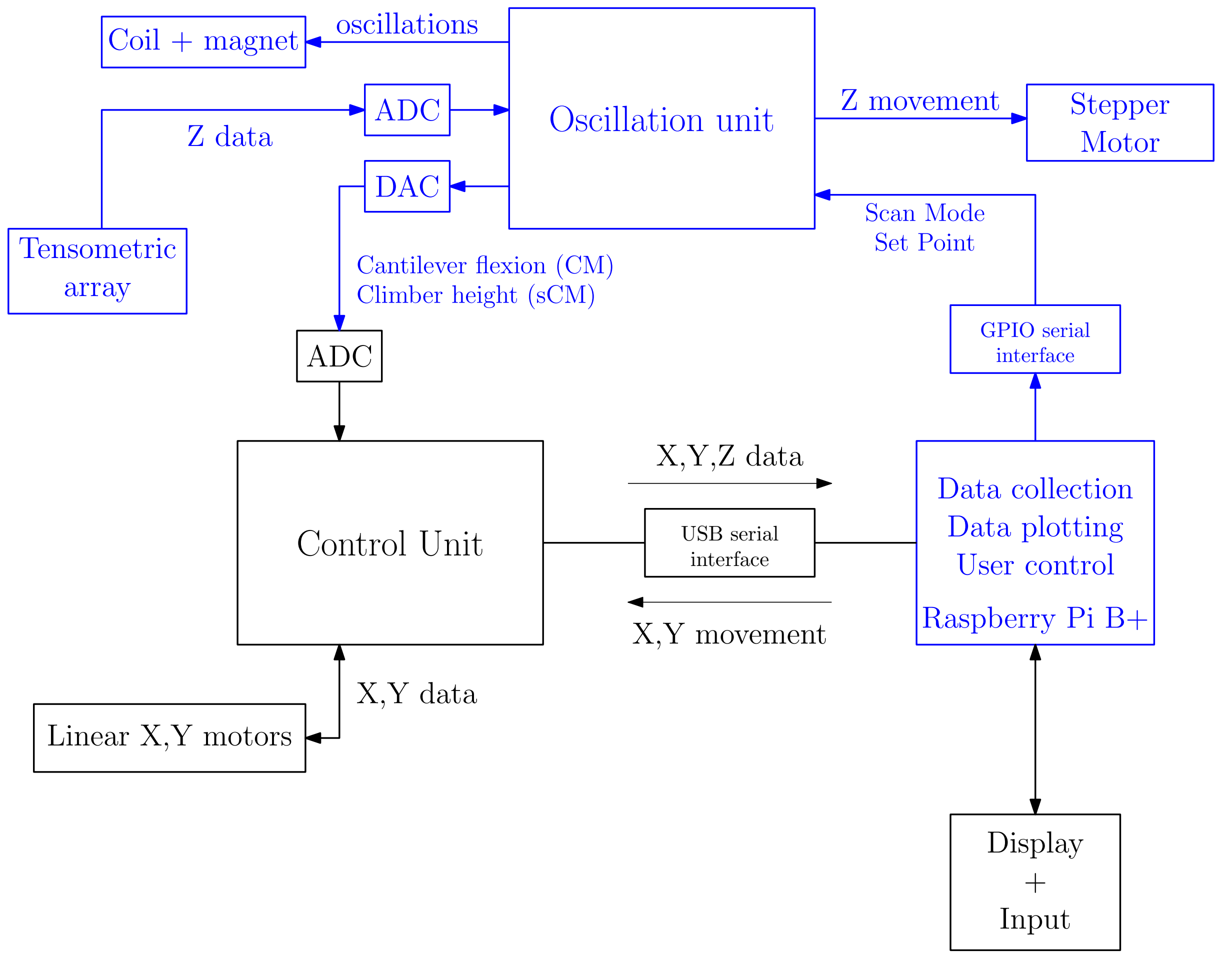


Figure 6.2: Schematic of the new model. All innovated components are marked in blue. Both custom printed circuit boards (PCBs) are controlled by a Raspberry Pi computer via serial communication interfaces. A new Oscillation unit was implemented to gather and analyse data from a tensometric array placed on the cantilever and control oscillations and vertical movement of the cantilever. This data is analysed, and afterwards sent to the control unit,[1] which combines it with information about position of sample and sends it to the Raspberry Pi computer, where it can be plotted and displayed.

[1]This ensures that there is minimal time delay between gathering Z data and combining it with X and Y data. Were the information sent directly to the Raspberry Pi, then the data would be sent via two different serial interfaces, not one. This could cause additional and unpredictable delays between signals in input/output buffers of these serial ports.

7. Construction

The original design of the cantilever is explained in Figure 7.1. Since it did not allow movement in the vertical axis, it had to be redesigned.

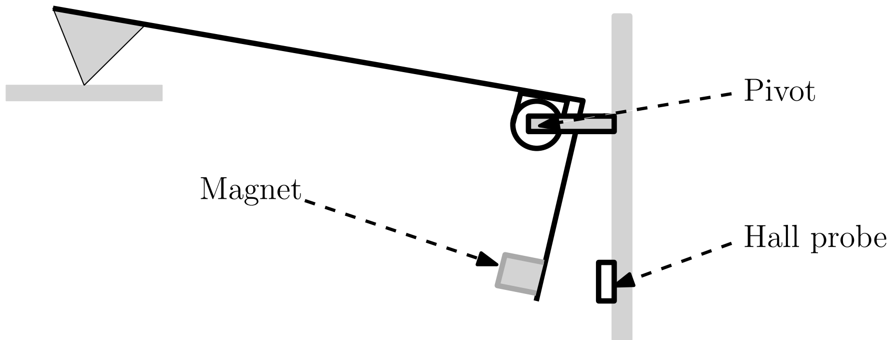


Figure 7.1: Original cantilever design. The change in height of sample turns the cantilever around the pivot and changes the distance between the magnet and the Hall probe.

New design is depicted in Figure 7.2. It allows the cantilever to move vertically and oscillate with a variable frequency. The magnet + Hall probe system used to detect vertical deflection of cantilever was replaced by a tensometric array placed directly on the cantilever.

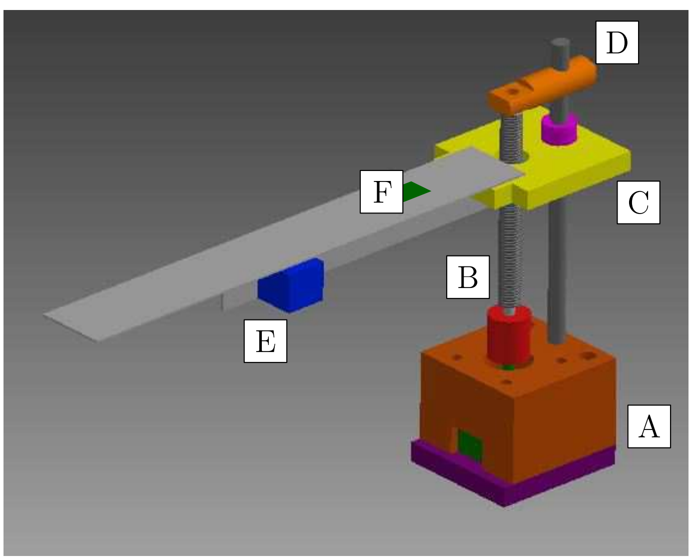


Figure 7.2: New design of the cantilever module. A stepper motor is anchored by a removable aluminum casing (A). The stepper motor turns the leadscrew (B), which causes the "climber" (C) to move up or down. The leadscrew is connected to a linear guide by a cap (D) which ensures their colinearity and locks the leadscrew in place. The cantilever is attached to the climber, and oscillations can be induced by a induction coil (E) and a magnet attached to the cantilever. A tensometric array (F) is attached to the cantilever to measure its vertical flexion.

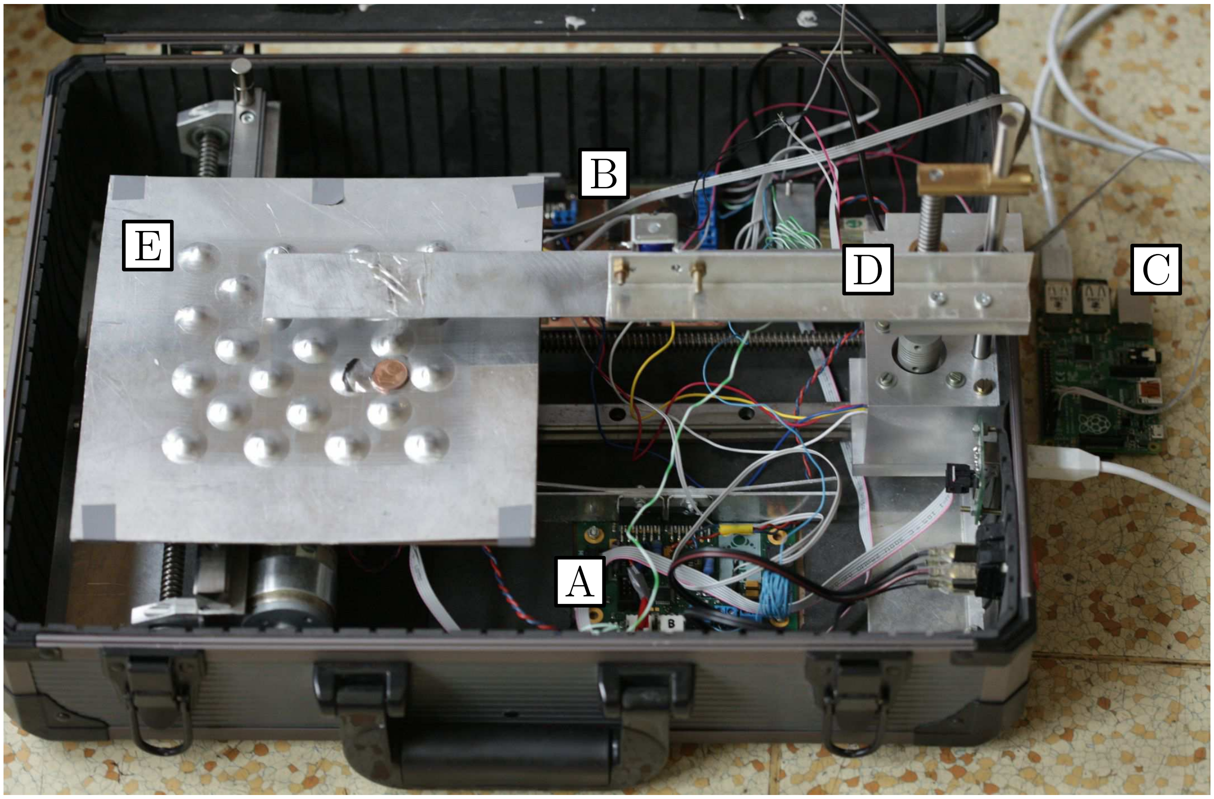


Figure 7.3: Photo of the new model. A - control unit, B - oscillation unit, C - Raspberry Pi, D - cantilever module, E - sample.

8. Electronics

The original model contained one custom-designed PCB (the control unit) for control and data collection. In the new design, one additional custom-designed PCB (the oscillation unit) and a Raspberry Pi model B+ single-board computer were implemented.

8.1. Oscillation unit

8.1.1. Function

An overview of the oscillation unit function is given in Figure 6.2. Just as the control unit, it is powered by an Atmega8 microcontroller and programmed in C programming language. It enables following functions:

- Scan mode selection - CM/sCM, CHM/CIM.[1]
- Vertical movement of cantilever.
- Induction of oscillations of cantilever with variable frequency and precision of $\pm 0{,}1$ Hz.
- Feedback loop for constant interaction mode - see Table 8.1.
- Gathering, processing and sending data - see Table 8.2.

8.1.2. Oscillations and feedback

Table 8.1: Set point variables in individual scanning modes.

	CHM	CIM
CM	–	Cantilever deflection
sCM	–	Oscillation amplitude

Table 8.2: Variables for data processing and plotting. These are the variables which are sent to the control unit as Z data.

	CHM	CIM
CM	Cantilever deflection	Climber height
sCM	Oscillation amplitude	Climber height

[1]For explanation of these individual modes, refer to Sections 2.4, 4.2 and 4.4.

Both extraction of oscillation amplitude from the signal from the tensometers and also feedback loop for constant interaction mode could be implemented either using electrical circuits or digitally. For purposes of this model, purely digital implementation was used. The reasons are following:

Extraction of oscillation amplitude from the signal could be carried out by an electronic circuit called the envelope detector – Figure 8.1. The time constant $\tau = RC$ of this circuit has to be tuned to suit the cantilever's oscillation frequency. In general, the time constant must fulfil the following equation [13]:

$$\frac{1}{f_{\mathrm{m}}} \gg \tau \gg \frac{1}{f_{\mathrm{c}}}, \tag{8.1}$$

where f_{m} is the highest modulation frequency of the signal (i.e. how fast the signal amplitude is changing), and f_{c} is the carrier frequency of the signal (i.e. frequency of cantilever oscillations). This means that if the cantilever is for any reason changed for one with a different oscillation frequency, this circuit would also have to be modified. Implementing envelope detection digitally is thus beneficial to flexibility of the model.

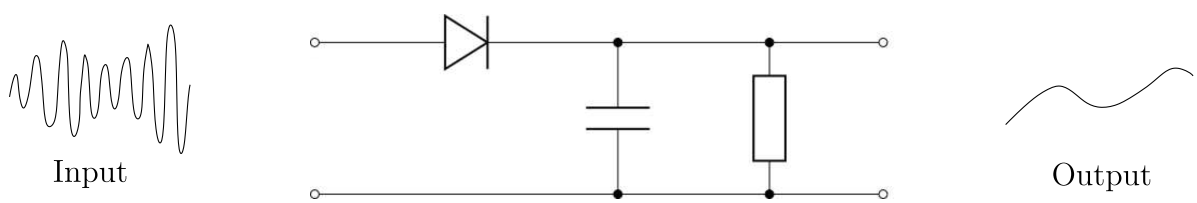


Figure 8.1: Envelope detector circuit schematic.

A feedback loop circuit would be much more complicated, since the stepper motor requires very specific values and characteristics of signals at each of its input wires. Controlling the feedback digitally makes it much easier to modify and again benefits the flexibility of the model.

8.2. Raspberry Pi Model B+

8.2.1. Function

The single-board computer integrated into the model is required for following tasks:

- Communication with and control of both custom PCBs (control and oscillation unit) via serial interfaces.
- Collection and analysis of recieved data.
- User control and data display in a graphical user interface.

All these tasks were originally carried out by the external Windows OS computer. After integration of the Raspberry Pi, only an external display and mouse+keyboard connection is required.[2] Controlling the device with a laptop (or a smartphone) is still

[2]Both of these devices can be also easily integrated into the model, at an estimated cost from 3000,- CZK upwards.

possible using a wireless or Ethernet connection and a VNC (Virtual Network Computing) program.

8.2.2. Software

Control software for the device was originally written in C#. This, as mentioned in Section 5.2, is unsuitable for Raspberry Pi. A different language, Python, was chosen for following reasons:

- It is a completely open language with a large user base.
- Its syntax is easy to learn and read – it is often recommended as a good first programming language for beginners.
- It is well-integrated with Linux and Raspberry Pi.
- It is an interpreted language – it does not require compilation before running and is easy to debug at runtime.
- Its large and powerful libraries (NumPy, SciPy, matplotlib) make it easy to analyse and visualise collected data.

Python also has its drawbacks, the most important one being speed. While it is still well-optimised, Python code cannot match similar code in C or other low-level languages. Fortunately, the Raspberry Pi Model B+ offers enough computational power to allow its use in this project.

Graphical user interface (GUI) was adapted from previous version of the device - Figure 8.2. It was designed using the GTK+ library and its main features were mentioned in Section 8.2.1.

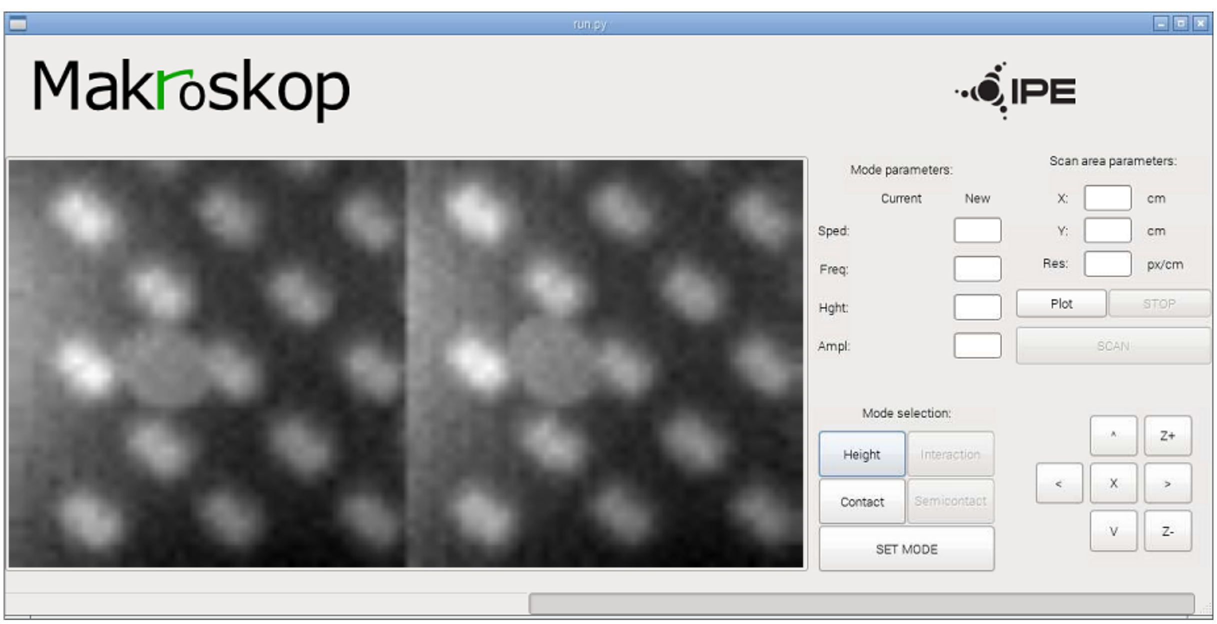


Figure 8.2: Graphical user interface of the device. It is used to control the device, set up scan parameters and display collected data.

9. Cantilever oscillations

Oscillation frequency of the cantilever is an important variable in every semicontact and noncontact AFM.

9.1. Free cantilever oscillations

Motion of a fixed-free oscillating cantilever (Figure 9.1) can be described with a fourth-order time-dependent partial differential equation [14]:

$$EI\frac{\partial^4 y}{\partial x^4} + \rho A\frac{\partial^2 y}{\partial t^2} = 0, \tag{9.1}$$

where $y(x,t)$ is the transverse deflection of the cantilever, E is the Young module of the cantilever, I is area moment of inertia, ρ is cantilever density and A is cantilever cross-section area.

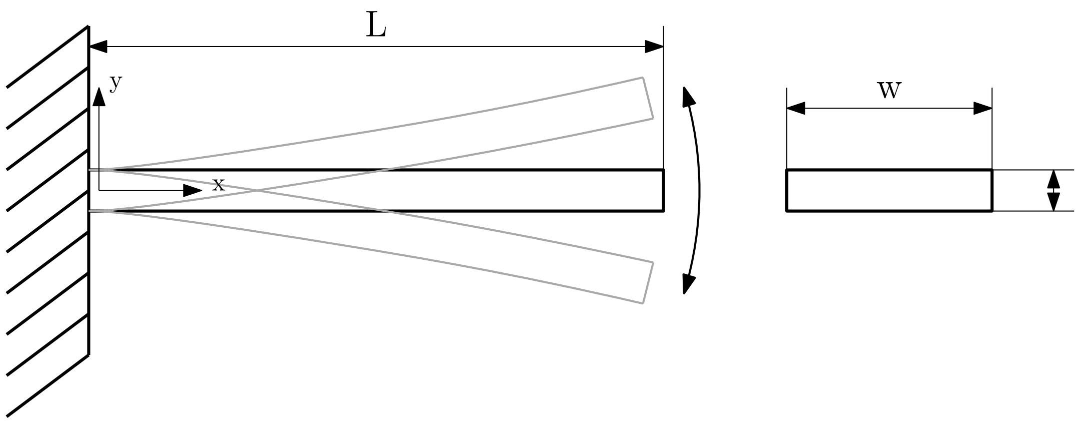


Figure 9.1: Fixed-free oscillating cantilever.

Solving this equation (for example in [15]) gives rise to these natural cantilever frequencies:

$$\omega_n = A_n\sqrt{\frac{EI}{\mu L^4}}, \tag{9.2}$$

where L is cantilever length, n is the number of oscillation mode, and A_n is a constant. For a fixed-free cantilever, values of A for first 3 modes are $A_1 = 3.52$, $A_2 = 22.0$ and $A_3 = 61.7$ [15].

By inserting cantilever dimensions and material characteristics into equation (9.2), we recieve the following resonance frequency:

$$f_1 = \frac{A_1}{2\pi}\sqrt{\frac{EI}{\mu L^4}} = \frac{A_1}{2\pi}\sqrt{\frac{Et^2}{12\rho L^4}} = \frac{3.52}{2\pi}\sqrt{\frac{2.1\times 10^{11}\,\mathrm{Pa}\times 0.49\,\mathrm{mm}^2}{12\times 7850\,\mathrm{kg\,m^{-3}}\times 53.1\,\mathrm{dm}^4}} \approx 8.0\,\mathrm{Hz} \tag{9.3}$$

9.2. Cantilever as a driven damped harmonic oscillator

If there are external forces acting on the cantilever, an additional term appears on the right side of equation (9.1). Solutions of this equation depend on characteristics of the external force and aren't trivial [16].

Instead, the cantilever can be modelled as a driven damped harmonic oscillator. Its equation of motion then becomes:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + 2\gamma \frac{\mathrm{d}y}{\mathrm{d}t} + \omega_0^2 y = f(t), \tag{9.4}$$

where ω_0 is the natural resonance frequency, γ is the damping factor and $f(t)$ is the driving force as a function of time.

9.2.1. Sinusoidal wave

Usually, the driving force has a sinusoidal shape:

$$f(t) = C \sin(\omega t), \tag{9.5}$$

where C is the amplitude and ω is the angular frequency of the driving force. The equation (9.4) can then be solved analytically [17], and the resonance curve[1] is displayed in Figure 9.3.

9.2.2. Square wave

In our model, time dependence of the driving force has the shape of a square wave - see Figure 9.2. A square wave with an amplitude C can be represented via a Fourier series as a linear combination of sinusoidal waves and a constant term:

$$f(t) = C \left(\frac{1}{2} + \frac{2}{\pi} \sum_{n=1,3,5...}^{\infty} \frac{\sin(n\omega t)}{n} \right), \tag{9.6}$$

The differential equation (9.4) becomes:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + 2\gamma \frac{\mathrm{d}y}{\mathrm{d}t} + \omega_0^2 y = \frac{F_0}{2} + \frac{2F_0}{\pi} \sum_{n=1,3,5...}^{\infty} \frac{\sin(n\omega t)}{n}, \tag{9.7}$$

where F_0 is the amplitude of the driving force. A resonant response from the oscillator should occur each time when the frequency $\omega_n = n\omega, n = 1, 3, 5...$ of one of terms from the sum is close to or equal to the resonant frequency ω_0 of the oscillator [18].

Resonance curves for a harmonic oscillator driven by a sinusoidal or a square wave – calculated using a numerical simulation – are displayed in Figure 9.3. The resonance response of cantilever used in the model is displayed in Figure 9.4.

[1]Dependence of steady-state oscillations amplitude on frequency of driving force.

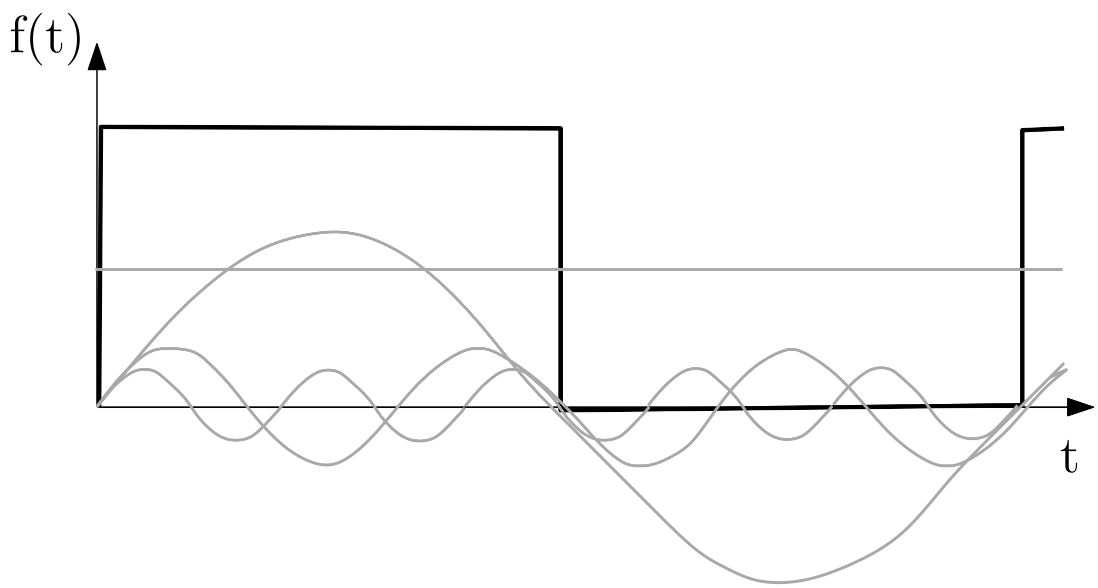


Figure 9.2: A square wave with its 4 most significant components (constant term, fundamental sine wave, third and fifth harmonics).

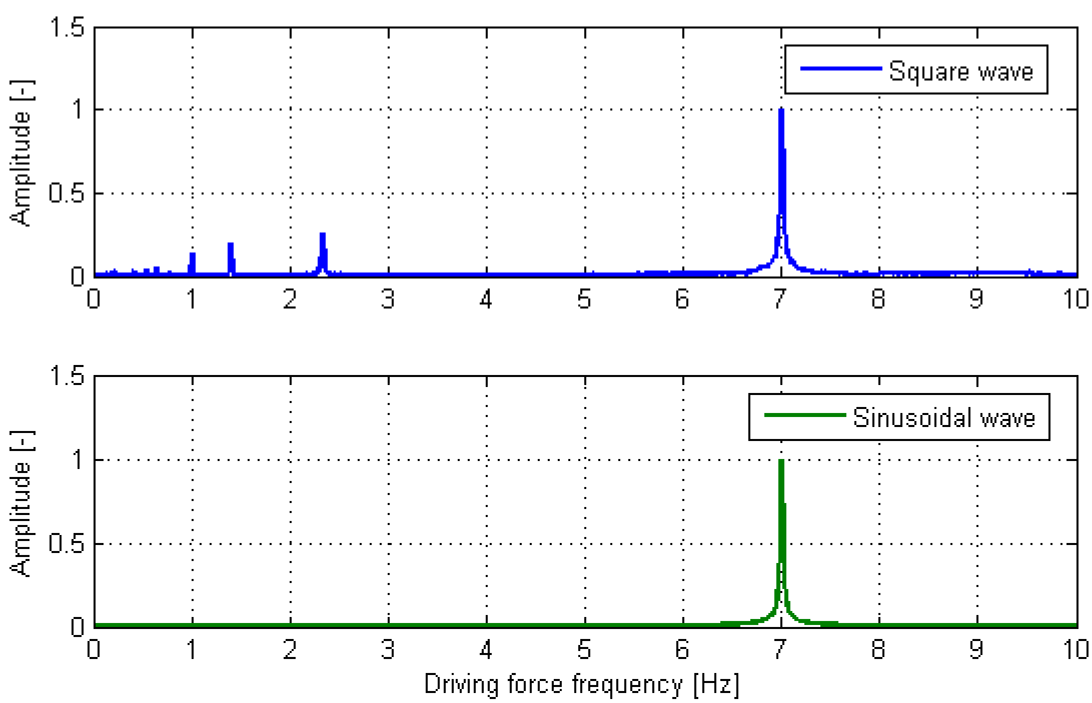


Figure 9.3: Resonance curves for a sinusoidal and square-wave driving force. Vertical axis units are arbitrary. $f_0 = 7\,\mathrm{Hz}$. Notice the extra peaks corresponding to resonance with higher hamonics of the square wave ($f = \frac{f_0}{n}, n = 1, 3, 5, ...$), which are absent in the resonance curve for a sinusoidal force.

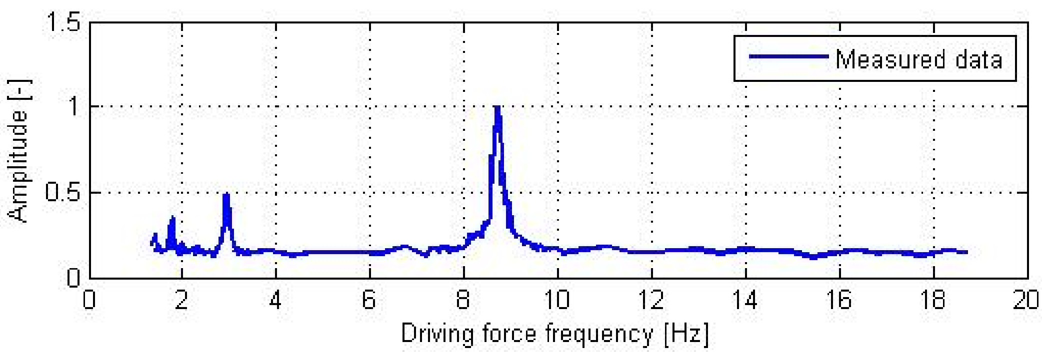


Figure 9.4: Measured resonance curve of the cantilever. Resonant frequency $f_0 = 8.7\,\mathrm{Hz}$. Extra peaks at frequencies ($f = \frac{f_0}{n}, n = 1, 3, 5, ...$) are present, just as the numerical model predicted.

10. Notable features

10.1. Development process

The development process of the model resembles in many ways development processes of actual scanning probe microscopes. First STMs and AFMs were contact mode (developed in 1981, resp. 1986) [19]. Noncontact AFM and semicontact AFM were developed subsequently in the next decade [20]. In our model, contact mode was also first to be developed, with semicontact mode implemented additionally.

10.2. Signal path

Another interesting similarity can be found in the design of oscillation unit. Between the cantilever and final display in the computer, the signal changes form between analog and digital several times using analog/digital and digital/analog converters (ADC and DAC) – see Figure 10.1. At first, the control unit received data directly from the probe, but later the data is first processed by the oscillation unit and then sent to the control unit. Similar features can be found in real AFMs: The Oscillation Controller 4 by company Specs Zurich also takes analog inputs and can produce analog outputs, but all internal data processing is purely digital:

> "With an analog bandwidth of 5 MHz the OC4 is wellsuited to operating at higher resonance modes. [...] Internal signals are represented at 32 bits with at least 1 MS/s. [...] Up to six analog outputs and two digital lines allow easy integration with any SPM controller." [21]

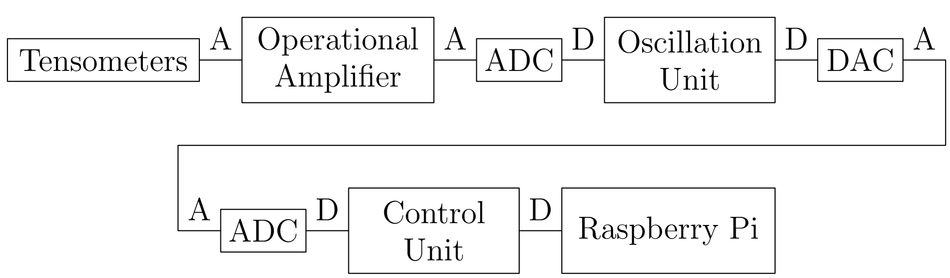


Figure 10.1: Path of signal from the cantilever to the Raspberry Pi computer. Signal changes form between analog (A) and digital (D) multiple times.

11. Conclusion

Purpose of this work was to improve an already-existing model of a scanning probe microscope by researching and implementing an additional suitable SPM technique, and removing the need for an external computer by implementing a single-board computer into the device.

Originally, the model only supported constant height contact mode of SPM. After researching and discussing multiple options, the model was modified to support four different SPM techniques – constant height and constant interaction mode, both of which can run in contact or semicontact mode. In Chapter 9, behaviour of oscillating cantilever was studied, with interesting results arising from simple analysis techniques such as harmonic approximation and Fourier analysis.

A single-board computer – Raspberry Pi model B+ – was implemented into the device. An external computer is now no longer necessary, although external input devices (mouse and keyboad) and output devices (display) are still required for operation. Use of open-source systems and popular programming languages made the device more flexible and user-friendly. Many features – for example enhanced data analysis or an analogy to individual atom manipulation – can be implemented in the future.

This model can not only serve as a great demonstration tool on science fairs and popular science lectures. It can also be useful to somebody, who wants to improve their practical skills such as programming, construction or designing electronic circuits. They can practice their knowledge and try out new ideas on a functional device without risking major damage or high production costs. This practical experience, which many scientists lack, can be invaluable later in their career, when they will be designing their own experiments and instruments.

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List of acronyms

- ADC – analog-to-digital converter
- AFM – atomic force microscopy
- CHM – constant height mode
- CIM – constant interaction mode
- CM – contact mode
- DAC – digital-to-analog converter
- GUI – graphical user interface
- MFM – magnetic force microscopy
- OS – operating system
- PCB – printed circuit board
- sCM – semicontact mode
- SCM – scanning capacitance microscopy
- SNOM – scanning near-field optical microscopy
- SPM – scanning probe microscopy
- STM – scanning tunnelling microscopy
- SThM – Scanning Theremin Microscope
- VNC – Virtual Network Computing